EXPANSION OF A FORMALISM OF CLASSICAL MECHANICS FOR NONEQUILIBRIUM SYSTEMS

V.M. Somsikov*
Laboratory of Physics of the geoheliocosmic relation, Institute of Ionosphere, Almaty, Kazakstan.
(Dated: February 2, 2008)

The expansion of a classical Hamilton formalism consisting in adaptation of it to describe the nonequilibrium systems is offered. Expansion is obtained by construction of formalism on the basis of the dynamics equation of the equilibrium subsystems by which the nonequilibrium system is represented. It has allowed removing restrictions on dynamics of the subsystems, which dictated by the requirement of monogenic and potentiality of the forces between subsystems. Modified Lagrange, Hamilton and Liouville equations are obtained. Some features of dynamics of nonequilibrium systems are considered. Connection between the equation of interaction of subsystems and a thermodynamic principle of energy is analyzed.

PACS numbers: 05.45; 02.30.H, J

I. INTRODUCTION

The attempts of further development of methods of researches of nonequilibrium systems collides with a problem of irreversibility [1-4]. The analysis of approaches to solution of this problem leads us to conclusion, that the one of the general reason of its difficulties is a restriction on the frameworks of formalisms of the classical mechanics. Really, creation of the organized structures is caused by the dissipations. But dissipation is not present in Hamilton systems because the obtaining of the Hamilton principle based on condition that the forces of interaction of systems are potentially and monogenic [5].

Necessity of expansion of formalisms of the classical mechanics have arisen as a result of investigating of dynamics of hard disks [6, 7]. Forces of interaction of hard disks systems are non-potential. Therefore it was necessary so to modify canonical Lagrange, Hamilton and Liouville equations that they have been applicable for the description of dynamics of non-potentially of interacting systems. Such modification consisted in obtaining of these equations basing on the D'Alambert principle under condition of non-potentiality of the forces [5]. From modified Liouville equation followed that nonpotentiality of collective forces of interacting of systems is a necessary condition of existence of irreversible dynamics [7].

In the nature all fundamental forces are potential. Therefore it was necessary to generalize results of researches of hard disks on systems of potentially interacting elements. For this purpose as a method of the description of dynamics of nonequilibrium systems we have taken advantage of an opportunity of representation of nonequilibrium systems as a set of equilibrium subsystems (ESS). This method of system's splitting on the ESS is not new. It was used with success at construction of statistical physics of equilibrium systems when interaction ESS can be neglected. But it follows from a condition of maximum entropy that ESS for nonequilibrium system will be in motion in relative to each other [8]. Therefore to determine their dynamics it is necessary to take into account the interaction between them. The equation of interaction of systems (UVS) for calculation of the ESS dynamics was obtained within the framework of classical mechanics [9]. Using UVS and basing on D'Alambert principle about equality to zero of a variation of work of effective forces, the modified Lagrange, Hamilton and Liouville equations for interaction ESS have obtained. These equations determine expansion of a formalism of the classical mechanics, allowing study of the open and nonequilibrium systems.

This paper is constructed as follows. The UVS and modified Lagrange, Hamilton and Liouville equations are obtained. The analysis of the important laws of dynamics of nonequilibrium systems and relation between classical mechanics and thermodynamics are submitted.

II. THE EQUATION OF ONE SYSTEM DYNAMICS

Let us show, how obtaining of the equations of dynamics of elements and their systems are possible. The equation of dynamics of two interacting systems will be obtained in a similar way.

Let us consider system of potentially interacting elements. If the system is conservative, we will have for energy E: $\dot{E} = 0$. The energy of the system depends on elements velocities, and their coordinates. Therefore we have: $E = E(r, v)$, where r, v are a set of coordinates and velocities of the particles. In this case the equality, $\dot{E} = 0$, takes place only when energy depends on two additive parts. One part should be a function of velocity, and the second one - coordinates. Then energy of the system can be presented as $E = \varphi[T + U] = const$, where $T = \sum_{i=1}^{N} T_i({v_i}^2)$, v_i is a velocity of i- element, T is the kinetic energy of the system, and $U(r_i)$ is the poten-

*Electronic address: nes@kaznet.kz

tial one [10]. The φ-function should be linear in order to be constant when the coordinates and velocities are being changed. It is always possible to represent such function as $E = T + U$ by means of scale transformation and usage of the necessary system of coordinates. So, the sum of kinetic and potential energies of the system in a non-homogeneous space should be constant.

Let us take a moving elementary particle with mass m and velocity v. The kinetic energy corresponding to the particle will be $T(v^2) = mv^2/2$, and the potential energy -$U(r)$, so $E = mv^2/2 + U(r) = const$. In this case from equality $\dot{E} = 0$ follows that:

$$v(m\dot{v} + \partial U/\partial r) = 0 \tag{1}$$

The eq. (1) is a balance equation of the kinetic and potential energies. As eq. (1) should be fulfilled in case of any direction of the vector velocity, the following requirement takes place:

$$m\dot{v} = -\partial U/\partial r \tag{2}$$

It is Newton equation (NE). This equation is determining the connection of acceleration of the particle with the external force. The right hand side of eq. (2) is the active force. The left hand side - is the inertial force [5]. The particle moves along the gradient of a potential function. During the motion of the particle along the closed line in a potential field, the work of forces is equal to zero. Therefore dynamics of the particle is reversible.

Let us take a system, which consists of N potentially interacting elements located in the non-homogeneous space; the mass of each element is equal to 1. The force acting on each element is equal to the sum of forces of all elements and the force caused by non-homogeneous space. The force between two elements is central and it depends on the distance between them.

Let us represent the energy of the system as a sum of kinetic energies of elements - $T_N = \sum_{i=1}^{N} m{v_i}^2/2$, potential energies in the field of external forces - ${U_N}^{env}$, and the potential energy of their interaction $U_N(r_{ij}) = \sum_{i=1}^{N-1}\sum_{j=i+1}^{N} U_{ij}(r_{ij})$, where v_i - is a velocity of i -element; $r_{ij} = r_i - r_j$ - is a distance between elements i and j. So, $E = E_N + U^{env} = T_N + U_N + U^{env} = const$. The time derivative of the energy will be as follows: $\dot{E} = \dot{E}_N + \dot{U}^{env}$, where $\dot{E}_N = \sum_{i=1}^{N} v_i(m\dot{v}_i + \sum_{j\neq i}^{N} F_{ij})$; $\dot{U}_{env} = \sum_{i=1}^{N} v_i F_i^{env}$; $F_{ij} = \partial U_N/\partial r_{ij}$, $F_i^{env}(r_i) = \partial U^{env}/\partial r_i$. So we have:

$$\sum_{i=1}^{N} v_i \tilde{F}_i = 0 \tag{3}$$

Where $\tilde{F}_i = m\dot{v}_i + \sum_{j\neq i}^{N} F_{ij} + F_i^{env}$ is effective force for i particle. Then the eq. (3) can be rewritten as: $\dot{E} = \sum_{i=1}^{N} v_i \tilde{F}_i = 0$. This equality can be treated as orthogonality of the vector of effective forces with respect to the vector of velocities of elements of the system. If there are no restrictions imposed on the v_i directions, the requirement $\tilde{F}_i = 0$ is satisfied [5]. Then from eq. (3) we obtain:

$$m\dot{v}_i = -\sum_{i=1}^{N} v_i \tilde{F}_i - F_i^{env} \tag{4}$$

It is NE for the system's elements in non-homogeneous space. The eq. (4) has coincided with the corresponding equation in [11] though it is obtained by other way.

Let us obtain an equation of motion of the system as a whole in an external field. It is known [10], that a motion of the system in the homogeneous space is characterized by two integrals: energy of motion of the center of mass and the total energy of motion of the particles inside of the system relative to the center of mass. We will name second energy as the internal energy of the system. Therefore it is reasonable to rewrite the eq. (3) having presented systems energy as the total of these two types of energies. For this purpose we can use the following equality: $T_N = \sum_{i=1}^{N} m{v_i}^2/2 = m/(2N)\{V_N^2 + \sum_{i=1}^{N-1}\sum_{j=i+1}^{N} v_{ij}^2\}$ (a), where $V_N = \dot{R}_N = 1/N\sum_{i=1}^{N} \dot{r}_i$ -are velocities of the center of mass; R_N - are coordinates of the center of mass; $v_{ij} = \dot{r}_{ij}$. We will write the energy of the system in such a way: $E_N = T_N^{tr} + E_N^{ins}$, $E_N^{ins} = T_N^{ins} + U_N$. Then the eq. (3) can be written as follows:

$$\dot{T}_N^{tr} + \dot{E}_N^{ins} = -\sum_{i=1}^{N} v_i F_i^{env} \tag{5}$$

Where $\dot{T}_N^{tr} = M_N V_N \dot{V}_N; M_N = mN$; $\dot{E}_N^{ins} = \dot{T}_N^{ins} + \dot{U}_N^{ins} = \sum_{i=1}^{N-1}\sum_{j=i+1}^{N} v_{ij}(m\dot{v}_{ij}/N + F_{ij})$.

The term $\dot{T}_N^{tr}$ in eq. (5) determines the change of the kinetic energy of motion of the system as a whole, and the term $\dot{E}_N^{ins}$ represents change of the internal energy. The right hand side determines the change of energy of the system as a result of action of external forces.

Let us to transfer to the generalized variables in eq. (5). For this purpose we will represent velocity of the motion of elements of the system as the sum of velocities of their motion with respect to the center of mass of the system - $\tilde{v}_i$, and velocity of the center of mass itself - V_N , i.e. $v_i = \tilde{v}_i + V_N$. Using these variables we will have the following: $T_N = \sum_{i=1}^{N} m{v_i}^2/2 = m/(2N)V_N^2 + mV_N\sum_{i=1}^{N}\tilde{v}_i + \sum_{i=1}^{N} m\tilde{v}_i^2/2$. As $\sum_{i=1}^{N}\tilde{v}_i = 0$, then

$T_N = m/(2N)V_N^2 + \sum_{i=1}^{N} m\tilde{v}_i^2/2$. Therefore $\sum_{i=1}^{N} m\tilde{v}_i^2/2 = 1/(2N)\sum_{i=1}^{N-1}\sum_{j=i+1}^{N} v_{ij}^2$. Thus the kinetic energy of the relative motion of particles of the system equals the sum of kinetic energies of the particles' motion with respect to the center of mass.

Let us take into account that $r_{ij} = \tilde{r}_{ij} = \tilde{r}_i - \tilde{r}_j$, where $\tilde{r}_i, \tilde{r}_j$ - are coordinates of the elements with respect to the center of mass of the system. So $U_N(r_{ij}) = U_N(\tilde{r}_{ij}) = U_N(\tilde{r}_i)$. That is $\sum_{i=1}^{N-1}\sum_{j=i+1}^{N} v_{ij}F_{ij}(r_{ij}) = \sum_{i=1}^{N} \tilde{v}_i F_i(\tilde{r}_i)$, where $F_i = \partial U_N/\partial\tilde{r}_i = \sum_{j\neq i, j=1}^{N} \partial U_N/\partial r_{ij}$. By means of generalization of corresponding equalities for the kinetic and potential energies of the system, we will obtain from eq. (5):

$$V_N M_N \dot{V}_N + \sum_{i=1}^{N} m\tilde{v}_i(\dot{\tilde{v}}_i + F(\tilde{r})_i) = \\ = -V_N F^{env} - \sum_{i=1}^{N} \tilde{v}_i F_i^{env}(R, \tilde{r}_i) \qquad (6)$$

Here $F^{env} = \sum_{i=1}^{N} F_i^{env}(R, \tilde{r}_i)$, R-is a coordinate of center of mass.

The eq. (6) determines the balance of energy of the system in non-homogeneous space. The first term in the left hand side corresponds to change of kinetic energy of motion of system as the whole. The second term determines the change of internal energy.

Let us take into account that $F^{env} = F^{env}(R + \tilde{r}_i)$, and suppose that $R \gg \tilde{r}_i$. Then it is possible to expand the force F^{env} in a series using a small parameter, $\tilde{r}_i/R$. Keeping the terms up to first-order of infinitesimal, we will have: $F_i^{env} = F_i^{env}|_R + (\nabla F_i^{env})|_R\tilde{r}_i \equiv F_{i0}^{env} + (\nabla F_{i0}^{env})\tilde{r}_i$. Taking into account that $\sum_{i=1}^{N} \tilde{v}_i = \sum_{i=1}^{N} \tilde{r}_i = 0$ and $\sum_{i=1}^{N} F_{i0}^{env} = NF_{i0}^{env} = F_0^{env}$, we can set from (6):

$$V_N(M_N\dot{V}_N) + \sum_{i=1}^{N} m\tilde{v}_i(\dot{\tilde{v}}_i + F(\tilde{r})_i) \approx \\ \approx -V_N F_0^{env} - (\nabla F_{i0}^{env})\sum_{i=1}^{N} \tilde{v}_i\tilde{r}_i \qquad (7)$$

The force F_0^{env} is potential and depends on R. The right hand side of eq.(7) determines the work of external forces. The first term is depending on the velocity of systems motion and coordinate of its center of mass. It is determine the change of kinetic energy of system as the whole.

The second term is depending on coordinates of particles and their velocities in relative to the center of mass. It is determine the change of internal energy of system. Thus, work of external forces is splitting on two essentially different parts.

The right hand side is the first order of infinitesimal, because despite $R \gg \tilde{r}_i$, it value are not small.

If the external field is homogeneous then $(\nabla F^{env})_{i0} = 0$. The variables in the eq. (7) is separating, and we have:

$$M_N\dot{V}_N = F_0^{env} \qquad (8)$$

$$m\dot{\tilde{v}}_i = -F(\tilde{r}_i)_i \qquad (9)$$

The eq. (8) is an equation of the motion of the system as a whole in an external field, and the eq. (9) is an equation of the motion of elements of the system. It follows from these equations, that in a homogeneous external field the kinetic energy of the system as a whole is variable only, and the internal energy is constant. The change of this kinetic energy does not depend on the forces between elements. The system is equivalent to the single body with the mass which is equal to the sum of masses of the particles. The motion of elements of the system does not depend on an external field and is determined by forces of interaction only.

Thus, the system of potentially interacting elements in an external field can be considered, us a structured particle. Generally the work of external forces changes both its internal energy, and energy of its movement. Therefore dynamics of such system (or the structured particle) is determined by the equation (6). When the heterogeneity of external forces can be neglected, dynamics of system is described by the Newton equation.

III. THE EQUATION OF INTERACTION OF TWO SUBSYSTEMS

Let us accept that the nonequilibrium system can be presented by set of moving relative to each other of ESS. For ESS a role of external forces carry out forces from other ESS. Obviously, it is impossible to neglect by heterogeneity of these forces in generally. Therefore dynamics ESS will be described by the equation (6) in which the external forces is a forces from other ESS. Hence, having replaced in (6) the right-hand side on these forces, we will obtain the UVS which describe the dynamics of nonequilibrium system. Let us show, how it is possible to obtain UVS.

Let us the system consists of two interacting equilibrium subsystems - L and K. Let us all elements to be identical and have the same weight 1, and L to be a number of elements in L - subsystem, K -is a number of elements in K -subsystem, i.e. $L + K = N$, $V_L = 1/L\sum_{i=1}^{L} v_i$ and $V_K = 1/K\sum_{i=1}^{K} v_i$ - are subsystems' velocities with respect to the center of mass. Let the velocity of the center of mass be equal to zero, i.e. $LV_L + KV_K = 0$.

We can represent the energy of the system as $E_N = E_L + E_K + U^{int} = const$, where E_L and E_K are the subsystems' energies, and U^{int} - is the energy of their interaction. According to the eq. (4), the energy of each subsystem can be represented as $E_L = T_L^{tr} + E_L^{ins}$, $E_K = T_K^{tr} + E_K^{ins}$, where $T_L^{tr} = M_L V_L^2/2$, $T_K^{tr} = M_K V_K^2/2$, $M_L = mL, M_K = mK$. E^{ins}- is the internal energy of a subsystem. The E^{ins} consists of the kinetic energy of motion of the elements with respect to the center of mass - T^{ins} and their potential energy - U^{ins}, i.e. $E^{ins} = T^{ins} + U^{ins}$, where $U_L^{ins} = \sum_{i_L=1}^{L-1} \sum_{j_L=i_L+1}^{L} U_{i_L j_L}(r_{i_L j_L})$, $U_K^{ins} = \sum_{i_K=1}^{K-1} \sum_{j_K=i_K+1}^{K} U_{i_K j_K}(r_{i_K j_K})$. The energy U^{int} is determined as $U^{int} = \sum_{j_K=1}^{K} \sum_{j_L=1}^{L} U_{j_L j_K}(r_{j_L j_K})$. Indexes j_k, j_L, i_K, i_L determine belonging of the elements to corresponding subsystem. In equilibrium $T^{tr} = 0$. Hence, if the system aspirates to equilibrium, then T^{tr} energy for each subsystem will be transformed into the internal energy.

We have obtained the equations of dynamics of L and K ESS in the following way. Let us differentiate energy of system on time. In order to find the equation for L - subsystem, at the left hand side of obtained equality we have kept only those terms which determine the change of the kinetic and potential energies of interaction of elements of L - subsystem. We replaced all other terms in the right hand side and combined the groups of terms in such a way when each group represents plurality of the terms forming the NE for K-subsystems elements. Therefore these groups are equal to zero. As a result the right hand side of the equation will be contain only the terms which determine the change of the potential energy of interaction of the elements L - subsystem with the elements K - subsystem. The equation for K - subsystem we will obtain in the same way. So we will have:

$\sum_{i_L=1}^{L} m v_{i_L} \dot{v}_{i_L} + \sum_{i_L=1}^{L-1} \sum_{j_L=i_L+1}^{L} v_{i_L j_L} F_{i_L j_L} = - \sum_{i_L=1}^{L} v_{i_L} F_{i_L}^K$ (b),

and for K-subsystem:

$\sum_{i_K=1}^{K} m v_{i_K} \dot{v}_{i_K} + \sum_{i_K=1}^{K-1} \sum_{j_K=i_K+1}^{K} v_{i_K j_K} F_{i_K j_K} = \sum_{j_K=1}^{K} v_{j_K} F_{j_K}^L$ (c).

Here $F_{i_L}^K(R_K, r_{i_L}) = \sum_{j_K=1}^{K} F_{i_L j_K}$, $F_{j_K}^L(R_L, r_{i_K}) = \sum_{i_L=1}^{L} F_{i_L j_K}$ - are forces between the corresponding particle of one ESS and all particles of the other ESS. The work of these forces determines the change of energy of ESS. $R_K = (1/K) \sum_{i_K=1}^{K} r_{i_K}$; $R_L = (1/L) \sum_{i_L=1}^{L} r_{i_L}$.

For obtaining from the equations (b, c) the equations of subsystems interaction, it is necessary to present their left-hand side in the form of two terms. One term should characterize the change of energy of a motion of a ESS as the whole, and second is a change of its internal energy. With this purpose let us take into account that velocities of the elements can be represented as the sum of their velocities with respect to the center of mass of the ESS and the velocity of the ESS with respect to the center of mass of the system, $v_i = \tilde{v}_i + V$. Then with a help of (a), we will obtain from (b, c):

$$V_L M_L \dot{V}_L + \sum_{i_L=1}^{L-1} \sum_{j_L=i_L+1}^{L} \{v_{i_L j_L} [\frac{m \dot{v}_{i_L j_L}}{L} + + F_{i_L j_L}]\} = -\Phi_L - V_L \Psi \qquad (10)$$

$$V_K M_K \dot{V}_K + \sum_{i_K=1}^{K-1} \sum_{j_K=i_K+1}^{K} \{v_{i_K j_K} [\frac{m \dot{v}_{i_K j_K}}{K} + + F_{i_K j_K}]\} = \Phi_K + V_K \Psi \qquad (11)$$

Here $\Psi = \sum_{i_L=1}^{L} F_{i_L}^K$, $\Phi_L = \sum_{i_L=1}^{L} \tilde{v}_{i_L} F_{i_L}^K$, $\Phi_K = \sum_{i_K=1}^{K} \tilde{v}_{i_K} F_{i_K}^L$.

The eqs. (10, 11) are equations of systems interaction (UVS). The first terms in the left hand side of UVS is a change of motion energy of ESS - "$\dot{T}^{tr}$", and the second terms is a change of their internal energy - "$\dot{E}^{ins}$".

The right hand side of UVS are consisting of two terms determining the work of collective forces of interaction ESS. The first terms, "Φ_L " and "Φ_K", determine the work of the interaction force on transformation of motion energy of ESS into their internal energy. The second terms include potential force, "Ψ". It is a central force which depends on distances between the centers of mass of ESS: $\Psi = \Psi(R_{LK})$, where $R_{LK} = R_L - R_K$. The work of "Ψ" determines the change of velocities of ESS. As well as in the case of the motion of the system in a non-homogeneous external field (see the eq. (7)), when $R_L \gg \tilde{r}_{i_L}$, $R_K \gg \tilde{r}_{i_K}$ this work can be estimated by expanding of force in a Taylor series.

It is possible to transform the equations (10, 11) to the form of the equations containing forces of friction. Let us take into account that $\sum_{i_L=1}^{L} m \tilde{v}_{i_l} \dot{\tilde{v}}_{i_L} = (1/L) \sum_{i_L=1}^{L-1} \sum_{j_L=i_L+1}^{L} m v_{i_L j_L} \dot{v}_{i_L j_L}$, $\dot{U}_L = \sum_{i_L=1}^{L} F_{i_L} \tilde{v}_{i_L} = \sum_{i_L=1}^{L-1} \sum_{j_L=i_L+1}^{L} F_{i_L j_L} \tilde{v}_{i_L j_L}$, $F_{i_L} = \sum_{j_L \neq i_L}^{L} \partial U_L / \partial \tilde{r}_{i_L}$. And for K -subsystem is similar. If also introduce the following designation: $\alpha_L = -(\dot{E}_L^{ins} + \Phi_L)/V_L^2$, $\alpha_K = -(\dot{E}_K^{ins} - \Phi_K)/V_K^2$, $\dot{E}_L^{ins} = \sum_{i_L=1}^{L} \tilde{v}_{i_L} (m \dot{\tilde{v}}_{i_L} + F_{i_L})$, $\dot{E}_K^{ins} = \sum_{i_K=1}^{K} \tilde{v}_{i_K} (m \dot{\tilde{v}}_{i_K} + F_{i_K})$ then the eqs. (10,11) can be rewritten as:

$$M_L \dot{V}_L = -\Psi - \alpha_L V_L \qquad (12)$$

$$M_K\dot{V}_K = -\Psi - \alpha_K V_K \qquad (13)$$

Here coefficients "α_L", "α_K" are equal to the ratio between the energy of motion and the full kinetic energy of correspondent ESS. Thus, the forces of interaction of the ESS are divided into the potential and non-potential parts, and α is a similar to the friction coefficient. The non-potential part of the force determined by coefficient corresponds to dissipation. It is important to note that here energy is not disappeared. Actually the value of energy is constant, but energy is redistributed between the elements of the subsystem. The eqs. (12, 13) are equivalent to the empirical motion equations for the structured particles.

Let us perform the following replacement: $V_L = KV_{LK}/N$, $V_K = -LV_{LK}/N$, where $V_{LK} = \dot{R}_{LK} \equiv V_L - V_K$. As the center of mass of the system is immovable, we will have from eqs.(10, 11):

$$\dot{E}^{tr}_{LK} + \dot{E}^{ins}_{L} + \dot{E}^{ins}_{K} = \Phi \qquad (14)$$

Here $\Phi = -\Phi_L + \Phi_K$, $\dot{E}^{tr}_{LK} = V_{LK}(M_R\dot{V}_{LK} + \Psi)$ - is the change of energy of the relative motion of the ESS, $M_R = mKL/N$.

The second and third terms in the eq. (14) determine the change of their internal energies. The right hand side determines the change of interaction energy. It is obvious that for an equilibrium system $\dot{E}^{tr}_{LK} = 0$. Then the eq. (14) is splitting on two independent equations for ESS.

We see that the work of the forces between ESS goes not only on change of their kinetic and potential energy, as in the case of elementary particles. It also goes on change of their internal energy. Therefore the force of interaction ESS represents the sum of two various forces. The first force determines motion of ESS as the whole as a result of mutual transformation their kinetic and potential energies. It is potential force. The second force determines the work on transformation of energy of interaction to the internal energy of ESS. It is non-potential force. This force does not change the momentums of ESS.

Thus, it is possible to consider equilibrium subsystems L and K as the structured particles. The motion of ESS are determined not only by transformations their kinetic and potential energy. But it is determined by the changes of their internal energy olso. Therefore the force of interaction ESS represents the sum of two various forces. The first force determines motion of ESS as the whole as a result of mutual transformation their kinetic and potential energies. It is potential force. The second force determines the work on transformation of motion energy into the internal energy of ESS. It is non-potential force. This force does not change the momentums of ESS.

If $L = 1$, $K = N - 1$ the equation (10) for L - subsystem will coincide with NE. The internal energy will be absent, and force acting on it will be potential. Therefore its dynamics is reversible. Therefore reversibility of dynamics of separate elements does not mean yet reversibility of dynamics of their systems. It is essential difference UVS from NE for elementary particles because in according with NE, the elementary particles return into initial points if the direction of velocity of their centers of mass will change on opposite, but ESS does not come back into initial points of their phase space when reversing them velocities.

Generally the potentials of interaction between particles inside ESS can be distinct from potentials of interaction of particles for different ESS.

IV. THE LAGRANGE, HAMILTON AND LIOUVILLE MODIFIED EQUATIONS

There is a question as in connection with the UVS the canonical Lagrange, Hamilton and Liouville are modified. The canonical equations follow from the integral principle of Hamilton [5, 14]. In turn the integral principle of Hamilton follows from differential principle of D'Alambert in case of potentiality of active forces between ESS. D'Alambert equation is formulated on the basis of NE.

In accordance with D'Alambert principle: "the work of the effective forces which includes the inertial and active forces is equal to zero for all reversible virtual displacements compatible with the restrictions given" [5]. For the closed non-equilibrium system that represents themselves by a set of the ESS, this principle will be as follows: the work of all forces of interaction of the ESS is equal to zero for all reversible virtual displacements compatible with the restrictions given.

If the change of the internal energy of ESS can be neglected, the work on their motion will be determined only by the potential part of interaction ESS forces. In this case instead UVS we can use NE and therefore come to the known canonical equations of a classical mechanics [5]. If the neglecting by the change of internal energy is impossible, D'Alambert equation should be written down on the basis UVS which take into account the distribution of the subsystems' motion energy as a whole between its internal energies in the result of the work of the non-potential part of forces.

Let us take a closed non-equilibrium system consisting of N elements which can be represented by a set of $R = 2$ an ESS. The modification of formalism is carried out by standard way [5]. Firstly, on the basis of UVS the D'Alambert equation is obtained. Based on it a principle of Hamilton, and then Lagrange equation are obtained. After that the Hamilton and Liouville equations for ESS are deduced.

If there are no external restrictions on system then the virtual displacements of the elements and ESS can be combined with the real ones [5]. As virtual work of all forces is determined by the eq. (14) we will have:

$$\delta\bar{W}_{LK} = \delta E^{tr}_{LK} + \delta E^{ins}_{L} + \delta E^{ins}_{K} + \delta\Phi = 0 \qquad (15)$$

The eq. (15) is D'Alambert equation for a non-equilibrium system. The first three terms in (15) deter-

mine the virtual change of energies of the ESS. The two last terms determine the virtual work for displacement of the elements of one ESS in the field of forces of the elements of the other ESS. I.e. they determine the change of internal energies of the ESS. The line above $\delta\bar{W}_{LK}$ means that it is just a differential form which does not come to a scalar function variation.

Let us transform the eq. (15) by means of multiplying by dt, and integrating from $t = t_1$ to $t = t_2$. As a result we will have:

$$\int_1^2 \delta\bar{W}_{LK}dt = \int_1^2 [\delta E^{tr}_{LK} + \delta E^{ins}_{L} + \delta E^{ins}_{K} + + \sum_{i_L=1}^{L} \delta\tilde{r}_{i_L} F_{i_L} - \sum_{i_K=1}^{K} \delta\tilde{r}_{i_K} F_{i_K}]dt = 0 \quad (16)$$

where $\delta\tilde{r}_{i_L}$ -is a virtual displacements of i_L element of L - subsystem; $\delta\tilde{r}_{i_K}$ - is a virtual displacements of i_K element of K- subsystem.

Let us rewrite the first three terms as follows: $\delta\int_1^2[\sum_{i_L=1}^{L} M_R V^2_{LK}/2 + U_{LK}]dt - [\sum_{i_L=1}^{L} M_R V_{LK}\delta R_{LK}]_{t_1}^{t_2}$; $\delta\int_1^2[\sum_{i_L=1}^{L} m\tilde{v}^2_{i_L}/2 + U_L]dt - [\sum_{i_L=1}^{L} m\tilde{v}_{i_L}\delta r_{i_L}]_{t_1}^{t_2}$; $\delta\int_1^2[\sum_{i_K=1}^{K} m\tilde{v}^2_{i_K}/2 + U_K]dt - [\sum_{i_K=1}^{K} m\tilde{v}_{i_K}\delta r_{i_K}]_{t_1}^{t_2}$;

The last two items in (16) are not the full differentials from any scalar function. I.e. in general it is impossible to represent the active forces of ESS interaction in the form of a gradient from a forcing function. Such forces are named as polygenic ones.

Let us the virtual displacements be equal to zero at the ends of the interval $[t_1, t_2]$. Then the eq. (16) can be rewritten as follows:

$$\delta S = \int_1^2 \delta\bar{W}_{LK}dt = \int_1^2 \{\sum_{n=1}^{N} [d/dt(\partial\Im/\partial v_n) - -\partial\Im/\partial r_n + F_n]\}\delta r_n dt \quad (17)$$

Here S- is action, $\Im = \sum_{n=1}^{N} [mv_n^2 + U_n]$ - is Lagrangian, $F_n = F_n^L - F_n^K$.

All variables are independent, and that is why in order to achieve simplification we have used through indexing for all elements of the system instead of indexing in accordance with the ESS, and at the same time new indexing is in accordance with the one accepted in the eq. (16). Thus, the action for a non-equilibrium system consists of the terms describing dynamics of the ESS as a whole, interior dynamics of the elements of the ESS and the term describing interaction of the ESS.

It follows from the requirement of independence of the generalized variables that

$$d/dt(\partial\Im/\partial v_n) - \partial\Im/\partial r_n = -F_n \quad (18)$$

This is the very modified Lagrange equation for a non-equilibrium system. The right hand side of the eq. (18) is equal to zero only when the relative motion of the ESS are absent. It should take place when the system is in equilibrium.

The eqs. (10, 11) were obtained by means of independent methods from the requirement of the system energy to be constant. It allows us to write the modified Lagrange equation for each of the ESS at once.

$$d/dt(\partial\Im_L/\partial v_{i_L}) - \partial\Im_L/\partial r_{i_L} = -F^K_{i_L} \quad (19)$$

$$d/dt(\partial\Im_K/\partial v_{i_K}) - \partial\Im_K/\partial r_{i_K} = -F^L_{i_K} \quad (20)$$

Here $\Im_L$ and $\Im_K$ - are Lagrange functions for the ESS.

Now let's obtain modified Hamilton equation. For $\Im$ the differential can be written as $d\Im = \sum_{n=1}^{N} [(\partial\Im/\partial v_n)dv_n + (\partial\Im/\partial r_n dr_n)] + \partial\Im/\partial t dt$. With the help of Legendry transformation, we will obtain: $d[\sum_{n=1}^{N} p_n v_n - \Im] = \sum_{n=1}^{N} [v_n dp_n - (\partial\Im/\partial r_n)dr_n] - (\partial\Im/\partial t)dt$. Since $\partial\Im/\partial t = -\partial H/\partial t$, where $H = d[\sum_{n=1}^{N} p_n v_n - \Im]$, we will have:

$$\partial H/\partial r_n = -\dot{p}_n - F_n \quad (21)$$

$$\partial H/\partial p_n = v_n \quad (22)$$

The above are modified Hamilton equations for a non-equilibrium system. The right hand side of the eq. (21) denotes non-potential forces. Modified Hamilton's equations for the ESS can be obtained in the same way.

Now let us obtain Liouville equations for the ESS and full system. For this porpoise let us take a generalized current vector $J_L = J_L(v_n, \dot{p}_n)$ of the L-subsystem (here "n" index corresponds only to the particles of the L-subsystem). From the eqs. (21, 22) we find: $divJ_L = \sum_{n=1}^{L} (\partial v_n/\partial r_n + \partial\dot{p}_n/\partial p_n) = -\sum_{n=1}^{L} \partial F_n^K/\partial p_n$. The continuity equation is a differential form of the particle number conservation law: $\partial f_L/\partial t + div(f_L J_L) = 0$, where $f_L = f_L(r, p, t)$ is a normalized distribution function for the elements of the L- subsystem. With the help of the continuity equation we will have: $df_L/dt = \partial f_L/\partial t + \sum_{n=1}^{L} (v_n \partial f_L/\partial r_n + \dot{p}_n \partial f_L/\partial p_n) = \partial f_L/\partial t + div(f_L J_L) - f_L divJ_L = -f_L divJ_L = f_L \sum_{n=1}^{L} \partial F_n^K/\partial p_n$. Thus we have:

$$df_L/dt = f_L \sum_{n=1}^{L} \partial F_n^L/\partial p_n \quad (23)$$

The eq. (23) is modified Liouville equation for the L -subsystem.

There is a formal solution of the eq. (23): $f_L = const \times \exp\int\{\sum_{n=1}^{L} \partial F_n^K/\partial p_n\}dt$. From this solution follows that the distribution function of a subsystem depends on time if force acting on the subsystem depends on velocities of the elements of the subsystem. It is similar result as for a hard disks systems [7].

The modify Liouville equation for system can be obtain from eqs. (21, 22) if $n = 1, 2...N$. We will have:

$$df_N/dt = f_N \partial F_n/\partial p_n \tag{24}$$

Despite absence of external forces for a system, the right hand side of the eq. (24) is not equal to zero. It is caused by the fact that the energy of subsystems' interaction does not include into ESS energy. Therefore the right hand side of the eq. (24) will not be equal to zero until the energy of interaction of the ESS is not transformed into their internal energy.

The reason of distinction between two descriptions of system (in a framework of canonical and modified equation) is the total work of potential forces between particles in the closed system is equal to zero. But the work on moving ESS is not equal to zero. The Newton equation for select particles can not determine this work. Therefore modified Lagrange, Hamilton and Liouville equations as against their canonical prototypes, are applicable for the description of dynamics of nonequilibrium systems.

V. SOME PROPERTIES OF DYNAMICS OF INTERACTING SUBSYSTEMS

In accordance with UVS, in order to describe a non-equilibrium system, the energy should be divided into T^{tr} and E^{ins}. As UVS includes the parameter describing the degree of non-equilibrium of a system, it allows studying evolution of the system. Let us to analyze some important cases of the system's dynamics.

In general case the non-potential forces can be rewritten as: $\Phi_L = \sum_{i_L=1}^{L} \Phi_{i_L}(R_K, \tilde{r}_{i_L}, \tilde{v}_{i_L})$, $\Phi_K = \sum_{i_K=1}^{K} \Phi_{i_K}(R_L, \tilde{r}_{i_K}, \tilde{v}_{i_K})$. If the sizes of ESS are less than the distances between them, we will have $\Phi_L \approx \sum_{i_L=1}^{L} F_{i_L}^K(R_K)\tilde{v}_{i_L} = F_{i_L}^K \sum_{i_L=1}^{L} \tilde{v}_{i_L} = 0$, and $\Phi_K \approx \sum_{i_K=1}^{K} F_{i_K}^L(R_L)\tilde{v}_{i_K} = F_{i_K}^L \sum_{i_K=1}^{K} \tilde{v}_{i_K} = 0$. In this case the eqs. (10, 11) are the Newton equations for two hard bodies. This case is similar to the case of homogeneity of an external field of forces.

In the case when $\Psi = 0$, $V_L = V_K = 0$, the first terms of the left side of UVS are equal to zero and the system is in equilibrium. The full energy of the system is equal to the sum of E^{ins} for each subsystem. Such system can be studied with the help of canonical Hamilton equations. ESS. Gibbs used this approach for creation of statistical mechanics of equilibrium systems [3, 11].

Now let us velocities of the elements with respect to the centers of mass of corresponding ESS be equal to zero during interaction of the ESS (this is a hard body approach). Then the right hand side, and also the second terms of left hand side of UVS are equal to zero, and UVS is transformed into NE for two hard bodies.

It is possible to come from classical mechanics to thermodynamics with the help of the UVS. Really, the right hand side of eqs. (10, 11) determines an change of ESS energy. The first term of the left hand side of UVS determines the change of the motion energy of ESS as the whole. In thermodynamics it corresponds to work, which is carried out by external forces acting on ESS on the part of an environment. The second term of the left hand side corresponds to increase in the entrance energy of a ESS. In thermodynamics this term corresponds to the change of thermal energy of ESS.

Let us consider the relation between the UVS and the basic equation of thermodynamics in details. We can write the basic equation of thermodynamics [8,13]: $dE = dQ - PdY$. Here, according to common terminology, E is energy of a ESS; Q is thermal energy; P is pressure; Y is volume. We take into account that $N >> 1, M_N = 1$. The energy change of the selected ESS is due to the work made by external forces. Therefore, the change in full energy of a subsystem corresponds to dE.

The change of kinetic energy of motion of a ESS as the whole, dT^{tr}, corresponds to the term PdY. Really, $dT^{tr} = VdV = V\dot{V}dt = \dot{V}dr = PdY$

Let us determine, what term in UVS corresponds to the change of the internal energy of ESS. As follows from virial theorem [10], if the potential energy is a homogeneous function of second order of the radiuses-vectors, then $\bar{E}^{ins} = 2\bar{\tilde{T}}^{ins} = 2\bar{\tilde{U}}^{ins}$. The line denotes the time average. Earlier we obtained that the energy, E^{ins}, increases due to T^{tr}. But the opposite process is impossible. Therefore the change of the term Q in the UVS corresponds to the change of the energy E^{ins}.

Let us consider the ESS near to equilibrium. If the ESS consist of N elements, the average energy of each element becomes, $\bar{E}^{ins} = E^{ins}/N = \kappa T_0^{ins}$. Now let the internal energy increases with dQ. According to the virial theorem, keeping the terms of the first order, we have: $dQ \approx T_0^{ins}[dE^{ins}/T_0^{ins}] = T_0^{ins}[dv/v_0]$, where v_0 is the average velocity of an element, and dv is its change. For ESS in equilibrium, we have $dv/v_0 \sim d\Gamma/\Gamma$, where Γ is the phase volume of a ESS, $d\Gamma$ will increase due to increasing of the ESS energy on the value, dQ. By keeping the terms of the first order we get: $dQ \approx T_0^{ins} d\Gamma/\Gamma = T_0^{ins} d\ln\Gamma$. By definition $d\ln\Gamma = dS^{ins}$, where S^{ins} is a subsystem entropy [9]. So, near equilibrium we have $dQ \approx T_0^{ins} dS^{ins}$. So formally

according with UVS the entropy production in the non-equilibrium system is determined by transformation of the motion energy of ESS into the internal energy. If it so eventually relative velocities of ESS go to zero. In result the energy of relative motion of ESS will be completely transforms into the internal energy and the systems equilibrates. It means that energy of motion of a ESS goes on increase of entropy. Therefore the deviation of entropy from equilibrium can be determined by the next formula [7]:

$$\Delta S = \sum_{l=1}^{R} \{ m_l \sum_{k=1}^{m_l} \int \sum_{s} \frac{F_{ks}{}^{m_l} v_k}{E^{m_l}} dt \} \qquad (25)$$

Here E^{m_l} is the kinetic energy of ESS; m_l is the number elements in ESS "l"; R is the number of ESS; s is number of the external element which collided with internal element k; $F_{ks}^{m_l}$ is a force, acted on element k-element; v_k -is a velocity of the k- element.

The formula (25) means, that a entropy production is provided by the energy of relative motion of ESS. It corresponds to entropy definition for the non-equilibrium systems, which was offered in [8].

But for informal connection of the equations of interaction of systems with thermodynamics, the increase of internal energy due to the energy of relative motion should be irreversible. Below some arguments for the benefit of such increase will be offered.

In connection with the law of momentum preservation of ESS the internal energy of the ESS is gradually increased due to energy $\dot{E}_{LK}^{tr}$. I.e. there is a gradual decrease of V_{LK}. To explain this fact let us take an equilibrium system and divide it into ESS. It follows from the requirement of equilibrium that the forces between the ESS are equal to zero. But if there are no external forces with respect to a subsystem, the subsystem cannot start moving. Indeed in this case the subsystem can start moving only due to its internal energy. But it is prohibited by the law of conservation of momentum of the subsystem. I.e. if the system is in equilibrium then it will be always remain in equilibrium state.

Now let us consider two interacting ESS which are in relative motion. The relative velocity of ESS can not be increased due to the energy of interaction of the ESS as this energy is itself determined by the relative velocities of the ESS. As well as in the previous case, this velocity can not be increased due to the internal energy of the ESS. So relative velocity can be decreased only.

It is follows from these arguments that UVS characterizes motion of system to an equilibrium state as a result of transition of energy of relative motion of ESS into internal energy. When system is in equilibrium, or when it is possible to freeze internal degrees of freedom of ESS, i.e. to neglect the change of their internal energy, then UVS is reduced to NE. Hence, it is possible to assert, that the broken of the time-symmetry of the systems dynamics is caused by the increasing of the internal energy. The decreasing of internal energy is prohibited by the law of conservation of momentum of the subsystem.

VI. CONCLUSION

Expansion of a formalism of classical mechanics and approach to the analysis of nonequilibrium systems are based on the key statement that closed non-equilibrium systems can be represented as a set of moving ESS [8]. This statement allowed transforming the tasks of dynamics of a non-equilibrium system to the tasks of dynamics of ESS. The offered approach has allowed removed the restrictions of applicability formalism of the classical mechanics, bound with the requirement of conservatism of systems. It has appeared enough for elimination of contradictions between a classical mechanics and thermodynamics.

Having expressed energy of system in the form of energy of a motion of ESS as the whole, their internal energies and energy of their interaction and differentiated it on the time, the UVS has been obtained. This equation is equivalent to the equation of structured particles.

In agreement with UVS the dynamics of ESS is determined by the collective force of their interaction. This force consists of two parts. The potential part is determining the transformation of the interaction energy into the motion energy of ESS. Non-potential force is determining the transformation of the ESS motion energy into internal energy. Thus, unlike dynamics of an elementary particle, the dynamics of ESS is determined by the work of interaction forces which will transform energy of interaction not only into potential and kinetic energy of ESS motion as the whole, how we have in the case of elementary particle, but also into the internal energy. Therefore based on NE which is valid only for elementary particles, it is impossible to describe the dynamics of the nonequilibrium system.

Based on UVS the modified Lagrange, Hamilton and Liouville equations was obtained. These equations are applicable to the study of dynamics of the open non-equilibrium systems because its have allowed taking into account the work of non-potential part of force on transformation of energy of ESS motion into their internal energy.

The following mechanism of irreversibility can be proposed: energy of ESS relative motion is transformed into their internal energy as a result of the work of the non-potential part of force of interaction of ESS. The decreasing of internal energy is prohibited by the law of conservation of momentum of the ESS. Therefore the system equilibrates, when relative motion of ESS is absent.

The explanation of the First law of thermodynamics is based on the fact that the work of subsystems' interaction forces changes both the energy of their motion and their internal energy. The explanation of the Second law of thermodynamics is based on the condition of irreversible transformation of the subsystems' relative motion energy into their internal energy.

The solution many problems are necessary for the further development of the offered approach to studying nonequilibrium systems and the strict proof of the conclusions offered here. Questions about the ways of splitting of nonequilibrium system on ESS, about character of transformation of energy of relative motion of ESS in their internal energy, etc., are the most important between them.

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